

“How do Electronic Laboratory Notebooks Inspire Researchers?”

Poster presentation at MAC/MLA (Mid-Atlantic Chapter / Medical Library Association)

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Virginia Tech University Libraries

Poster in VTechWorks institutional repository: <http://hdl.handle.net/10919/56951>

Selected References

Full reference list of literature review citations can be found in this Zotero Group and Library:

https://www.zotero.org/groups/electronic_laboratory_notebooks

General Reviews and Discussion of ELN

Bedford, E. (2013). Electronic Lab Notebooks | GradHacker | *Inside Higher Ed*. Retrieved October 17, 2015, from <https://www.insidehighered.com/blogs/gradhacker/electronic-lab-notebooks>

Kloeckner, F., Farkas, R., & Schmitz-Rode, T. (2012). The ELN-survey: On the potential of laboratory IT systems to support the biomedical research process. *Biomedizinische Technik*, 57(SUPPL. 1 TRACK-N), 776-779. doi: 10.1515/bmt-2012-4346. <http://www.degruyter.com/view/j/bmte.2012.57.issue-s1-N/bmt-2012-4346/bmt-2012-4346.xml>

Machina, H. K., Wild, D. J., Dey, P., & Merchant, M. (2013). Effective Integration of Informatics Tools to Enhance the Drug Discovery Process. *Industrial & Engineering Chemistry Research*, 52(47), 16547-16554. doi: 10.1021/ie401934a. <http://jla.sagepub.com/content/18/4/264.long>

Klokrose, C. N., & Zander, P. O. (2010). *Rethinking Laboratory Notebooks*. http://coop.wineme.fb5.uni-siegen.de/proceedings2010/8_cKlokrose_et_al_119_140.pdf

Rubacha, M., Rattan, A. K., & Hosselet, S. C. (2011). A Review of Electronic Laboratory Notebooks Available in the Market Today. *Journal of Laboratory Automation*, 16(1), 90-98. doi: 10.1016/j.jala.2009.01.002. http://www.slas.org/default/assets/file/2012_jala_readers_choice_award.pdf

Smith, C. (2014). Go Paperless with These Electronic Lab Notebooks. BioCompare. Retrieved October 17, 2015, from <http://www.biocompare.com/Editorial-Articles/158438-Go-Paperless-with-These-Electronic-Lab-Notebooks/>



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Historical Interest

(a few samples from the early years in ELN interest and development)

Finman, J., Fram, D. M., Kush, T., & Russell, C. H. (1983). An electronic laboratory notebook for VAX, PDP-11, and Professional 350 [microcomputers]. *DEC Professional*, 2(6), 120, 122, 124. "The main features of RS/1 are its user-friendliness and its integrated capabilities. Computer-naive engineers and scientists are taught RS/1's basic data-handling techniques in a few hours, after which they are ready to enter, manipulate, and analyze their own data using simple English commands and without having to write programs."

Fozard, A. (1977). Laboratory computer systems. *Laboratory Equipment Digest*, 15(8), 22-23. "The recently developed low price minicomputers and microprocessors allow modern product development laboratories to have 'thinking' electronic notebooks to help with the increasing workload arising from public demand for safety of manufactured products."

Martz, D. (1993). Implementing an electronic notebook data entry system at Hudson Foods. *Scientific Computing & Automation*, 9(11), 15-16. "In the staff's analysis, the Palm Top had five important characteristics. It used Lotus 1-2-3, a familiar industry standard with the ability to import and export data to many other applications. Its small size and light weight made it unobtrusive on the work bench and it was portable enough to fit into a chemist's smock pocket. It was durable and Hewlett Packard had a reputation as a dependable manufacturer. Moreover there were support programs and utilities available from third party companies. Finally, its 1 MB of memory was more than enough to hold daily test data until it could be downloaded each evening."

Themes

Research Data Management

Macdonald, S., & Macneil, R. (2015). Service Integration to Enhance Research Data Management: RSpace Electronic Laboratory Notebook Case Study. *International Journal of Digital Curation*, 10(1), 163-172. doi: 10.2218/ijdc.v10i1.354. <http://www.ijdc.net/index.php/ijdc/article/view/10.1.163/389>

Riedl, D. H., & Dunn, M. K. (2013). Quality assurance mechanisms for the unregulated research environment. *Trends in Biotechnology*, 31(10), 552-554. doi: 10.1016/j.tibtech.2013.06.007. <http://www.ncbi.nlm.nih.gov/pubmed/24054820>

Zimmerman, M. D., Grabowski, M., Domagalski, M. J., Maclean, E. M., Chruszcz, M., & Minor, W. (2014). Data management in the modern structural biology and biomedical research environment. *Methods in molecular biology (Clifton, N.J.)*, 1140, 1-25. doi: 10.1007/978-1-4939-0354-2_1. <http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4086192/>

Regulatory requirements

Weinberg, S., & Fuqua, R. (2011). A quick guide to ELN regulatory requirements. *Scientific Computing*, 28(6), 6-8. <http://www.scientificcomputing.com/articles/2012/05/quick-guide-eln-regulatory-requirements>

Industry examples

Elliott, M. H. (2012). The de-evolution of informatics: How externalization workflow is impacting traditional data management architectures. *Scientific Computing*, 29(5), 7-10.

<http://www.atriumresearch.com/library/SCI20121001%20Devolution%20of%20Informatics%20M%20Elliott.pdf>

Elliott, M. H. (2012). Structuring data management for ELN in formulations: S88 and S95 standards are excellent foundations for building an integrated platform. *Scientific Computing*, 29(6), 8-12.

<http://www.atriumresearch.com/library/SC Dec 2012 Structuring Data mgt for ELN Formulations.pdf>

Segalstad, S. H. (2011). Data management considerations for the environmental lab. *Scientific Computing*, 28(1), 6-9.

<http://www.scientificcomputing.com/articles/2011/05/data-management-considerations-environmental-lab>

Related - Exchangeable data formats

Lancashire, R., & Davies, A. I. M. (2013). The ACS 2013 symposium on exchangeable data formats.

Spectroscopy Europe, 25(5), 22-23+26. [Includes one or more programs on ELN specifically, but also related to integration / collaboration / sharing capabilities.]

<http://www.spectroscopyeurope.com/articles/tony-davies-column/3314-the-ac-s-2013-symposium-on-exchangeable-data-formats>

Metadata / Semantic Searching / Data Mining

Willoughby, C., Bird, C. L., Coles, S. J., & Frey, J. G. (2014). Creating Context for the Experiment Record. User-Defined Metadata: Investigations into Metadata Usage in the LabTrove ELN. *Journal of Chemical Information and Modeling*, 54(12), 3268-3283. doi: 10.1021/ci500469f.

<http://pubs.acs.org/doi/pdfplus/10.1021/ci500469f>

Yang, C., Tarkhov, A., Maruszyk, J., Bienfait, B., Gasteiger, J., Kleinoeder, T., . . . Rathman, J. (2015). New publicly available chemical query language, CSRML, to support chemotype representations for application to data mining and modeling. *Journal of Chemical Information and Modeling*, 55(3), 510-528. doi:

10.1021/ci500667v. <http://pubs.acs.org/doi/abs/10.1021/ci500667v>

Collaboration

(While these two examples focus on collaboration, this is also a topic discussed in most other articles and postings on ELN, including other references in this handout.)

Shoup, R. E., Beato, B. D., Pisek, A., White, J., Branstrator, L., Bousum, A., . . . Grever, T. (2013). Implementation of an electronic laboratory notebook to accelerate data review in bioanalysis. *Bioanalysis*, 5(13), 1677-1689. doi: 10.4155/bio.13.138. <http://www.ncbi.nlm.nih.gov/pubmed/23822130>

McCarthy, J. (2009). Enterprise lab notebook improves collaboration: Flexibility to partner can shorten path to more robust, promising pipeline. *Scientific Computing*, 26(4), 10-12.

<http://accelrys.com/micro/notebook/documents/SciCo-ELN-mccarthy-julaug09.pdf>

Research Literature

(Incorporation of research literature was occasionally mentioned in other articles, but this example places a strong focus on its usefulness as included within ELN usage.)

Khan, A. M., Hahn, J. D., Cheng, W.-C., Watts, A. G., & Burns, G. A. P. C. (2006). NeuroScholar's electronic laboratory notebook and its application to neuroendocrinology. *Neuroinformatics*, 4(2), 139-161. doi: 10.1385/NI:4:2:139. <http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4476904/>

Selected ELN Products

(Noted as used by or of interest for academic research, including a few major industry research ELN.)

Poster table in Google Sheets: <http://bit.ly/1NhGqHC>

Directory / Listing of ELN (including additional products to those listed below in this handout)

LiMSwiki.org - The laboratory, health, and science informatics encyclopedia, "ELN Vendors," http://www.limswiki.org/index.php/ELN_vendor

CERF ELN (Also RSpace and eCAT)

Elliott, M. H. (2009). What you should know before selecting an ELN. *Scientific Computing*, 26(3), E2-E10. <http://www.scientificcomputing.com/articles/2009/05/what-you-should-know-selecting-eln>

Macdonald, S., & Macneil, R. (2015). Service Integration to Enhance Research Data Management: RSpace Electronic Laboratory Notebook Case Study. *International Journal of Digital Curation*, 10(1), 163-172. doi: 10.2218/ijdc.v10i1.354. <http://www.ijdc.net/index.php/ijdc/article/view/10.1.163/389>

*RSpace discussion included

Contur ELN - Accelrys - BIOVIA

Contur ELN from Accelrys Powers UK's Largest Trial of Academic Electronic Lab Notebooks. (2012). *Technology News Focus*, 179. <http://www.prnewswire.com/news-releases/contur-eln-from-accelrys-powers-uks-largest-trial-of-academic-electronic-lab-notebooks-152767055.html>

Evernote

Walsh, E., & Cho, I. (2013). Using Evernote as an Electronic Lab Notebook in a Translational Science Laboratory. *Journal of Laboratory Automation*, 18(3), 229-234. doi: 10.1177/2211068212471834. <http://jla.sagepub.com/content/18/3/229.long>

E-Workbook

Denny-Gouldson, P., & Randle, E. (2009). Knowledge Management and Efficiency Gains. *American Laboratory*, 41(10), 9-+. <http://www.americanlaboratory.com/914-Application-Notes/562-Knowledge-Management-and-Efficiency-Gains/>

Beato, B., Pisek, A., White, J., Grever, T., Engel, B., Pugh, M., . . . Shoup, R. (2011). Going paperless: implementing an electronic laboratory notebook in a bioanalytical laboratory. *Bioanalysis*, 3(13), 1457-1470. doi: 10.4155/bio.11.117. http://www.future-science.com/doi/abs/10.4155/bio.11.117?url_ver=Z39.88-2003&rft_id=ori:rid:crossref.org&rft_dat=cr_pub%3dpubmed

Rajaroo, J., & Weiss, S. (2011). Using E-WorkBook Suite to implement quality control in real time: expanding the role of electronic laboratory notebooks within a bioanalysis laboratory. *Bioanalysis*, 3(13), 1513-1519. doi: 10.4155/bio.11.144. http://www.future-science.com/doi/abs/10.4155/bio.11.144?url_ver=Z39.88-2003&rft_id=ori:rid:crossref.org&rft_dat=cr_pub%3dpubmed

LabArchives

Bogdan, K., & Flowers, T. (2014). Electronic Lab Notebooks: Supporting Laboratory Data in the Digital Era. *Issues in Science & Technology Librarianship*(76), 2-2. doi: 10.5062/F4V9861X. <http://www.istl.org/14-spring/app.html>

Puccinelli, J. P., & Nimunkar, A. J. (2014). *An experience with electronic laboratory notebooks in real- World, client-based BME design courses*. Paper presented at the 121st ASEE Annual Conference and Exposition: 360 Degrees of Engineering Education, June 15, 2014 - June 18, 2014, Indianapolis, IN, United states. <http://www.asee.org/public/conferences/32/papers/9589/view>

LabTablet

Amorim, R. C., Castro, J. A., Rocha da Silva, J., & Ribeiro, C. (2014). *Labtablet: Semantic metadata collection on a multi-domain laboratory notebook*. Paper presented at the 8th Research Conference on Metadata and Semantics Research, MTSR 2014, November 27, 2014 - November 29, 2014, Karlsruhe, Germany. http://link.springer.com/chapter/10.1007%2F978-3-319-13674-5_19

LabTrove

Badiola, K. A., Bird, C., Brocklesby, W. S., Casson, J., Chapman, R. T., Coles, S. J., . . . Ylloja, P. M. (2015). Experiences with a researcher-centric ELN. *Chemical Science*, 6(3), 1614-1629. doi: 10.1039/c4sc02128b. <http://pubs.rsc.org/en/content/articlepdf/2015/sc/c4sc02128b>

Day, A. E., Coles, S. J., Bird, C. L., Frey, J. G., Whitby, R. J., Tkachenko, V. E., & Williams, A. J. (2015). ChemTrove: Enabling a Generic ELN To Support Chemistry through the Use of Transferable Plug-ins and Online Data Sources. *Journal of Chemical Information and Modeling*, 55(3), 501-509. doi: 10.1021/ci5005948. <http://pubs.acs.org/doi/pdfplus/10.1021/ci5005948>

Frey, J. G., Milsted, A., Michaelides, D., & De Roure, D. (2013). MyExperimentalScience, extending the 'workflow'. *Concurrency and Computation: Practice and Experience*, 25(4), 481-496. doi: 10.1002/cpe.2922. <http://onlinelibrary.wiley.com/doi/10.1002/cpe.2922/epdf>

Milsted, A. J., Hale, J. R., Frey, J. G., & Neylon, C. (2013). LabTrove: A Lightweight, Web Based, Laboratory "Blog" as a Route towards a Marked Up Record of Work in a Bioscience Research Laboratory. *PLoS One*, 8(7), e67460. doi: 10.1371/journal.pone.0067460 <http://journals.plos.org/plosone/article?id=10.1371/journal.pone.0067460>

Willoughby, C., Bird, C. L., Coles, S. J., & Frey, J. G. (2014). Creating Context for the Experiment Record. User-Defined Metadata: Investigations into Metadata Usage in the LabTrove ELN. *Journal of Chemical Information and Modeling*, 54(12), 3268-3283. doi: 10.1021/ci500469f.
<http://pubs.acs.org/doi/pdfplus/10.1021/ci500469f>

Yang, C., Tarkhov, A., Maruszczyk, J., Bienfait, B., Gasteiger, J., Kleinoeder, T., . . . Rathman, J. (2015). New publicly available chemical query language, CSRML, to support chemotype representations for application to data mining and modeling. *Journal of Chemical Information and Modeling*, 55(3), 510-528. doi: 10.1021/ci500667v

LabWare

Elliott, M. H. (2012). ELN in the bioanalytical laboratory. *Scientific Computing*, 29(1), 8-11.
<http://www.atriumresearch.com/library/SC%20Feb%202012%20ELN%20in%20the%20Bioanalytical%20Laboratory.pdf>

Specialized ELN or LIMS (Laboratory Information Management Systems) related to Molecular Biology / Bioinformatics / Health / Biomedical / Medicine research

ELN for Biologics

Elliott, M. H. (2013). The new frontier of biologics ELN. *Scientific Computing*, 30(5), 4-9.
<http://www.atriumresearch.com/library/FINALSCI20130801.pdf>

EMEN2

Rees, I., Langley, E., Chiu, W., & Ludtke, S. J. (2013). EMEN2: An Object Oriented Database and Electronic Lab Notebook. *Microscopy and Microanalysis*, 19(1), 1-10. doi: 10.1017/S1431927612014043.
<http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3907281/>

Rees, I., Mann, D., Damodaran, H., To, H., & Ludtke, S. J. (2007). EMEN2 - An extensible object oriented electronic lab notebook. *Biophysical Journal*, 530A-530A.

E-Workbook for Biology (IDBS)

Denny-Gouldson, P., & Randle, E. (2009). Knowledge Management and Efficiency Gains. *American Laboratory*, 41(10), 9-+. <http://www.americanlaboratory.com/914-Application-Notes/562-Knowledge-Management-and-Efficiency-Gains/>

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Nanotechnology (experimental product in development)

Mikolajczyk, M. M., Uchronski, M., Mowinski, K., Lubimow, M., Bijak, S., Teodorczyk, M., . . . Tykierko, M. (2014). Auxiliar Experimentorum - An Innovative Approach for Creating and Deploying Scientific Applications *eScience on Distributed Computing Infrastructure. Achievements of PLGrid Plus Domain-Specific Services and Tools: LNCS 8500* (pp. 211-225). Cham, Switzerland: Springer International Publishing.

NeuroScholar

Khan, A. M., Hahn, J. D., Cheng, W.-C., Watts, A. G., & Burns, G. A. P. C. (2006). NeuroScholar's electronic laboratory notebook and its application to neuroendocrinology. *Neuroinformatics*, 4(2), 139-161. doi: 10.1385/NI:4:2:139. <http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4476904/>

PiMS

Morris, C. (2015). PiMS: a data management system for structural proteomics. *Methods in molecular biology* (Clifton, N.J.). http://link.springer.com/protocol/10.1007%2F978-1-4939-2230-7_2#page-1